BENZYL 2-BROMOACETATE

Other names:	Benzyl bromoacetate
	Acetic acid, bromo-, phenylmethyl ester
	Acetic acid, bromo-, benzyl ester
	Bromoacetic acid, benzyl ester
Inchi:	InChI=1S/C9H9BrO2/c10-6-9(11)12-7-8-4-2-1-3-5-8/h1-5H,6-7H2
InchiKey:	JHVLLYQQQYIWKX-UHFFFAOYSA-N
Formula:	C9H9BrO2
SMILES:	O=C(CBr)OCc1ccccc1
Mol. weight [g/mol]:	229.07

Physical Properties

Property code	Value	Unit	Source
hf	-263.42	kJ/mol	Cheméo Relay (1.0)
hfus	21.18	kJ/mol	Joback Method
hvap	64.29	kJ/mol	Cheméo Relay (1.0)
ie	9.01	eV	Cheméo Relay (1.0)
log10ws	-2.62		Cheméo Relay (1.0)
logp	2.125		Crippen Method
mcvol	138.850	ml/mol	McGowan Method
pc	3736.23	kPa	Joback Method
tb	536.92	K	Cheméo Relay (1.0)
tf	277.59	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.03	J/mol×K	574.45	Joback Method
cpg	303.67	J/mol×K	612.88	Joback Method
cpg	314.52	J/mol×K	651.31	Joback Method
cpg	324.59	J/mol×K	689.74	Joback Method
cpg	333.94	J/mol×K	728.17	Joback Method
cpg	342.57	J/mol×K	766.60	Joback Method
cpg	350.54	J/mol×K	805.03	Joback Method
dvisc	0.0019077	Pa×s	349.57	Joback Method

dvisc	0.0011445	Pa×s	387.05	Joback Method
dvisc	0.0007515	Pa×s	424.53	Joback Method
dvisc	0.0005283	Pa×s	462.01	Joback Method
dvisc	0.0003915	Pa×s	499.49	Joback Method
dvisc	0.0003026	Pa×s	536.97	Joback Method
dvisc	0.0002418	Pa×s	574.45	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	441.20	K	2.90	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5437456&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature

tbrp: Boiling point at reduced pressure

tf: Normal melting (fusion) point